sp3s* Tight-Binding Parameters for Transport Simulations in Compound Semiconductors

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Abstract

A genetic algorithm approach is used to fit orbital interaction energies of sp3s* tight-binding models for the nine binary compound semiconductors consistent of Ga, Al, In and As, P, Sb at room temperature. The new parameters are optimized to reproduce the bandstructure relevant to carrier transport in the lowest conduction band and the highest three valence bands. The accuracy of the other bands is sacrificed for the better reproduction of the effective masses in the bands of interest. Relevant band edges are reproduced to within a few meV and the effective masses deviate from the experimental values typically by less than 10%.

KEYWORDS: sp3s* tight-binding, genetic algorithm, effective mass

1. Introduction

Nano-scaled electronic devices are characterized by material and charge density variations on the length scale of a few atoms. Tight-binding models [1] can resolve spatial material variations on an atomic scale and they bear the full crystalline and electronic symmetry of semiconductor materials in them. This ability has led to an increased use of these tight-binding models for the simulation of nano-scaled electronic devices (see references in [2]). While the tight binding approach is systematically appealing, it bears a big problem in that the basic building constructs for the tight-binding Hamiltonian are not conduction band edges and effective masses, but orbital interaction energies (15 "free" parameters in the sp3s* model). These interaction energies are related to the global bandstructure and effective masses in a non-trivial manner [3].

It is important to realize that the tight-binding models do not include all the physics of electronic structure. The accuracy of these models strongly depends on the choice of orbitals that are included and the parameterization of the orbital interaction energies. It is for example understood, but not widely appreciated, that the sp3s* nearest neighbor model pathologically predicts an infinite transverse mass at the X point [3]. With the limitations of the sp3s* model in mind it must be emphasized that early parameterizations [1] provided more global band structure fits for bands which can be probed by optical measurements. The complication in the fitting process of the 15 orbital interaction energies to measurable quantities has led to the use of the seminal Vogl [1] parameters in areas they were not

intended for. For example, quantitative electron transport simulations in high performance resonant tunneling diodes [4] require the proper representation of relative bandenergies as well as band curvature of the conduction *and* valence bands, even for a purely electronic device (no hole transport).

2. Method and Results

To enable an automated fitting of the orbital interaction energies to measureable quantities such as masses and band edges a genetic algorithm based procedure has been developed [2]. At the core of this algorithm is a single valued fitness function comprised of weighted standard deviations that are to be minimized for a list of bandstructure properties. The details of this algorithm are documented in reference [2]. The strength of the algorithm is its ability to search for global minima in a very nonlinear search space. In the course of this work it was verified that derivative-based search algorithms will get stuck in local minima.

The target material properties were taken from references [1, 5, 6]. Reported experimental material properties were preferred over theoretical values. The split-off band parameters Δ were restricted to be within a window of $\pm 30\%$ of the parameters listed by Vogl [1]. Note that the Vogl parameterization does not include these paramters and therefore does not model the split-off bands properly. The other orbital interaction energies were allowed to float free in energy. The interaction energies are normalized such that the valence band edge at Γ corresponds to 0 eV. The fitting for the nine binary compounds was performed in nine independent procedures. That implies that the on-site energies of one constituent vary from compound to compound. The new sp3s* parameters are listed in Table 1 to five decimal digits accuracy in units of eV.

Table 1: Bandstructure model parameters. All energies are in units of eV and the lattice constant is in units of nm.

Parameter	GaAs	AlAs	InAs	GaP	AlP	InP	GaSb	AlSb	InSb
lattice/(nm)	0.56660	0.56600	0.60583	0.54509	0.54635	0.58687	0.60959	0.61355	0.60583
$E(s,a)$	-3.53284	-3.21537	-9.57566	-8.63163	-8.93519	-7.91404	-7.16208	-4.55720	-7.80905
$E(p,a)$	0.27772	-0.09711	0.02402	0.77214	1.13009	0.08442	-0.17071	0.01635	-0.14734
$E(s,c)$	-8.11499	-9.52462	-2.21525	-1.77800	0.06175	-2.76662	-4.77036	-4.11800	-2.83599
$E(p,c)$	4.57341	4.97139	4.64241	4.17259	4.55816	4.75968	4.06643	4.87411	3.91522
$E(s^*,a)$	12.33930	12.05550	7.44461	11.90050	12.82470	9.88869	7.32190	9.84286	7.43195
$E(s^*,c)$	4.31241	3.99445	4.12648	7.99670	9.41477	7.66966	3.12330	7.43245	3.54540
$V(s,s)$	-6.87653	-8.84261	-5.06858	-7.21087	-6.68397	-6.16976	-6.60955	-6.63365	-4.89637
$V(x,x)$	1.33572	-0.01434	0.84908	1.83129	2.28630	0.75617	0.58073	1.10706	0.75260
$V(x,y)$	5.07596	4.25949	4.68538	4.87432	5.12891	4.23370	4.76520	4.89960	4.48030
$V(sa,pc)$	2.85929	2.42476	2.51793	6.12826	9.44286	3.62283	3.00325	4.58724	3.33714
$V(sc,pa)$	11.09774	13.20317	6.18038	6.10944	5.93164	6.90390	7.78033	8.53398	5.60426
$V(s^*a,pc)$	6.31619	5.83246	3.79662	6.69771	10.08057	4.61375	4.69778	7.38446	4.59953
$V(pa,s^*c)$	5.02335	4.60075	2.45537	6.33303	4.80831	6.18932	4.09285	6.29608	-2.53756
Δ_a	0.32703	0.29145	0.38159	0.05379	0.04600	0.09400	0.75773	0.70373	0.85794
Δ_c	0.12000	0.03152	0.37518	0.21636	0.01608	0.54000	0.15778	0.03062	0.51000

The resulting bandstructure properties are compared to the target properties in Tables 2 and 3. If no target value is listed, no "trusted" experimental or theoretical values could be found in references [1, 5, 6]. Just a few remarks relating to and beyond the results posted in Tables 2 and 3 are given due to space limitations. The light hole mass is more easily fit in small gap materials, where the magnitude of the conduction band to split-off hole band coupling is greater than that of the light hole to conduction bands [3]. Conduction band minima and longitudinal masses near the X-point on the Δ line are fitted for a several materials. Note that the sp3s* model breaks down as noted and visualized in references [2, 3] and no attempts have been made to fit the transverse electron mass at that minimum point. Only nominal weights are associated with the longitudinal L-point mass. No weight is given to the transverse L-point mass. During the fitting process it was observed that the upper conduction bands will be pushed unphysically close to the first conduction band if only effective masses and bandedges of the lowest conduction and three highest valence bands are considered. Including the Γ_{7c}, L_{7c} and X_{7c} with higher than nominal weights

keeps the upper conduction bands well above the lowest conduction band. The agreement with the L_{6c} value must be driven towards cautiously as a minima on the Λ line starts to develop instead of the minimum at the L point.

Table 2: Material properties (target and tight binding (TB) computed with parameters in Table 1) for GaAs, AlAs, InAs, GaP, and AlP grouped into properties at Γ, X, L and other spectrally accessible bands. Properties at Γ, and band edges at X and L received the highest weights. The other spectrally accessible bands are weighed only nominally except for Γ_{7c}, L_{7c} and X_{7c}.

Property	GaAs Target	GaAs TB	AlAs Target	AlAs TB	InAs Target	InAs TB	GaP Target	GaP TB	AlP Target	AlP TB
Γ_{6c}	1.424	1.424	3.020	3.018	0.370	0.368	2.780	2.779	3.620	3.620
Δ_{so}	0.340	0.312	0.300	0.291	0.380	0.381	0.080	0.080	0.040	0.040
m^*_Γ	0.067	0.068	0.150	0.154	0.024	0.024	0.077	0.219		0.249
$m^*_{lh}[001]$	-0.087	-0.080	-0.163	-0.151	-0.027	-0.028	-0.162	-0.160	-0.211	-0.184
$m^*_{lh}[011]$	-0.080	-0.073	-0.140	-0.131	-0.026	-0.027	-0.138	-0.142		-0.164
$m^*_{lh}[111]$	-0.079	-0.072	-0.135	-0.127	-0.026	-0.027	-0.133	-0.138	-0.145	-0.159
$m^*_{hh}[001]$	-0.403	-0.389	-0.516	-0.520	-0.345	-0.364	-0.448	-0.494	-0.513	-0.552
$m^*_{hh}[011]$	-0.660	-0.663	-1.098	-1.100	-0.639	-0.657	-0.853	-0.809		-0.864
$m^*_{hh}[111]$	-0.813	-0.838	-1.570	-1.578	-0.876	-0.883	-1.119	-0.982	-1.372	-1.026
m^*_{so}	-0.150	-0.159	-0.240	-0.262		-0.098	-0.465	-0.248		-0.279
Δ_{min}	$\approx$0.90	0.860	$\approx$0.75	0.800		1.000	$\approx$0.90	0.784	1.000	1.000
E^Δ_c	1.900	1.900	2.170	2.171	2.280	2.345	2.272	2.272	2.505	2.505
m^*_{Xl}	1.300	1.301	1.100	1.006		1.103	0.910	0.910		3.052
m^*_{Xt}	0.230	3.990	0.190	2.009		inf	0.254	2.265		inf
L_{6c}	1.708	1.708	2.352	2.351	1.500	1.460	2.637	2.635	3.570	3.540
m^*_{Ll}	1.900	1.775	1.900	2.609		1.852		24.323		>100
m^*_{Lt}	0.075	0.713	0.096	0.860		0.304		2.306		<0
Γ_{6v}	-13.100	-13.072	-11.950	-15.758	-12.300	-12.159	-12.300	-13.189	-11.820	-12.493
Γ_{7c}	4.530	4.312	4.540	3.994	4.390	4.126	4.870	4.845	5.090	5.687
Γ_{8c}	4.716	4.865	4.690	4.950	4.630	4.543	4.920	5.035	5.090	5.709
X_{5v}	-6.800	-4.710	-5.690	-4.064	-6.600	-7.595	-7.070	-7.876	-7.000	-6.085
X_{6v}	-2.880	-3.151	-2.410	-2.591	-2.400	-2.948	-2.730	-2.703	-2.270	-2.572
X_{7v}	-2.800	-3.023	-2.410	-2.449	-2.400	-2.836	-2.730	-2.678	-2.270	-2.555
X_{6c}	1.980	1.932	2.229	2.285	2.300	2.345	2.350	2.432	2.505	2.505
X_{7c}	2.320	2.117	3.800	2.461	2.500	2.849	2.750	2.651	4.300	4.461
L_{5v}	-8.000	-5.168	-6.000	-4.606	-6.230	-7.062	-6.840	-7.452	-6.000	-6.222
L_{6v}	-1.420	-1.528	-0.880	-0.956	-1.200	-1.399	-1.100	-1.320	-1.000	-1.253
L_{7v}	-1.200	-1.340		-0.782	-0.900	-1.144	-1.100	-1.254	-1.000	-1.228
L_{7c}	5.470	3.246	5.860	3.362	5.400	3.713	5.740	3.868	6.000	4.738

Table 3: Same as Table 2 for InP, GaSb, AlSb, and InSb.

Property	InP Target	InP TB	GaSb Target	GaSb TB	AlSb Target	AlSb TB	InSb Target	InSb TB
Γ_{6c}	1.344	1.345	0.750	0.751	2.300	2.300	0.169	0.169
Δ_{so}	0.108	0.105	0.760	0.747	0.673	0.675	0.858	0.847
m^*_Γ	0.077	0.078	0.041	0.042	0.120	0.121	0.014	0.014
$m^*_{lh}[001]$	-0.096	-0.082	-0.050	-0.043	-0.123	-0.099	-0.015	-0.014
$m^*_{lh}[011]$	-0.087	-0.076	-0.046	-0.040	-0.100	-0.089	-0.015	-0.014
$m^*_{lh}[111]$	-0.085	-0.075	-0.045	-0.040	-0.091	-0.086	-0.015	-0.014
$m^*_{hh}[001]$	-0.474	-0.480	-0.285	-0.300	-0.336	-0.363	-0.278	-0.287
$m^*_{hh}[011]$	-0.933	-0.886	-0.551	-0.559	-0.500	-0.632	-0.525	-0.531
$m^*_{hh}[111]$	-1.300	-1.187	-0.763	-0.759	-0.872	-0.800	-0.737	-0.732
m^*_{so}	-0.120	-0.150		-0.134	-0.290	-0.196		-0.132
Δ_{min}	$\approx$0.90	0.900	$\approx$0.80	0.850	$\approx$0.80	0.849		1.000
E^Δ_c	2.304	2.312	1.180	1.181	1.615	1.615	1.493	1.524
m^*_{Xl}		5.985	1.510	1.424	1.800	1.576		1.181
m^*_{Xt}		11.452	0.220	3.183	0.260	2.734		inf
L_{6c}	1.954	1.958	0.832	0.833	2.211	2.211	0.931	0.930
m^*_{Ll}		2.588	0.950	1.421		24.866		1.838
m^*_{Lt}		0.636	0.110	0.405		1.125	0.090	0.312
Γ_{6v}	-11.000	-12.025	-12.000	-12.683	-11.100	-10.975	-11.730	-10.814
Γ_{7c}	4.640	4.527	3.400	3.123	3.740	5.075	3.370	3.545
Γ_{8c}	4.920	5.055	4.700	4.033	4.000	5.135	3.740	3.703
X_{5v}	-6.010	-8.957	-6.760	-8.010	-6.760	-6.995	-6.430	-7.498
X_{6v}	-2.090	-2.440	-3.000	-3.433	-3.000	-3.192	-2.450	-3.190
X_{7v}	-2.060	-2.392	-2.500	-3.107	-2.500	-2.858	-2.240	-2.890
X_{6c}	2.304	2.314	1.400	1.210	1.615	1.632	1.493	1.524
X_{7c}	2.970	2.913		1.396	3.020	2.614	1.830	2.038
L_{5v}	-5.840	-7.774	-6.250	-7.689	-6.250	-7.160	-5.920	-7.054
L_{6v}	-1.090	-1.054	-1.450	-1.682	-1.450	-1.613	-1.400	-1.698
L_{7v}		-0.942	-1.000	-1.249	-1.000	-1.225	-0.900	-1.165
L_{7c}	5.580	4.232	4.400	2.432	4.400	3.476	4.000	2.969

3. Summary and Acknowledegement

This work provides a new parameterization of the widely used sp3s* tight binding model for the nine binary compounds consisting of In, Ga, Al and Sb, As, P. The new parametrization is expected to be more suitable for nanaloelectronic transport simulations than the seminal work by Vogl et al [1] since it focusses on the accuate modeling of effective masses and central bandedges. This is, to our knowledge, the first attempt to systematically fit anisotropic hole masses at Γ as well as electron masess at Γ and X.

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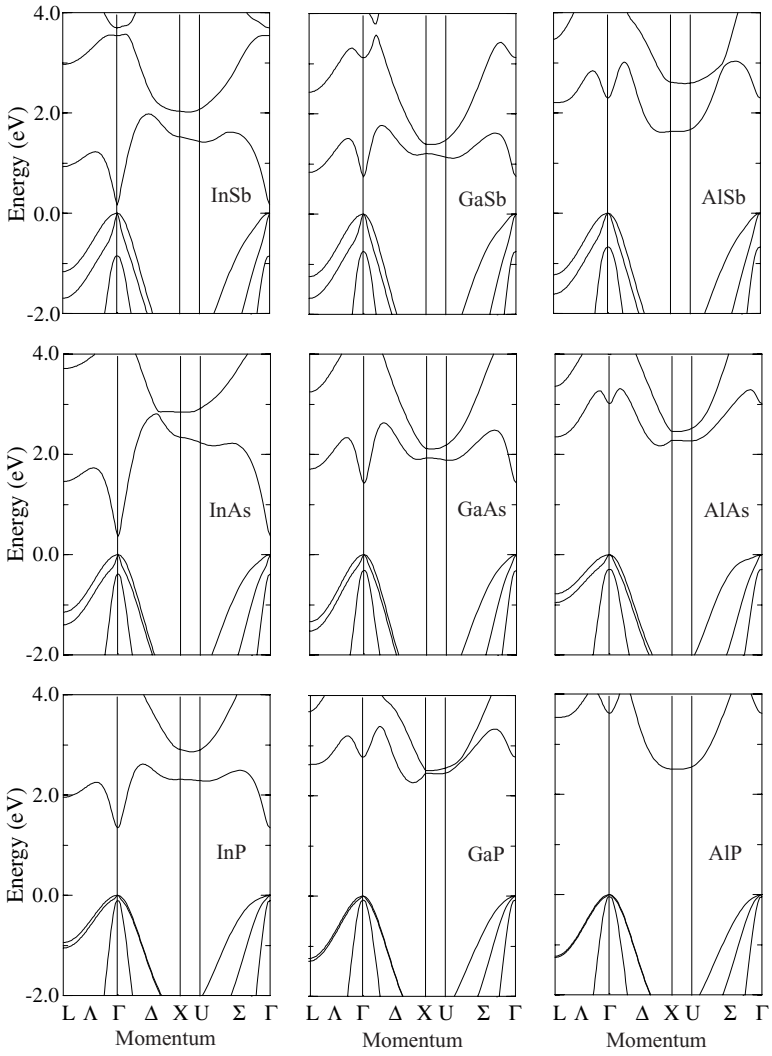

Figure 1: Dispersion relations for nine binary semiconductor compounds computed with the parameters listed in Table 1.

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